

Double-Well Optical Lattices with Atomic Vibrations and Mesoscopic Disorder

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Abstract

Double-well optical lattice in an insulating state is considered. The influence of atomic vibrations and mesoscopic disorder on the properties of the lattice are studied. Vibrations lead to the renormalization of atomic interactions. The occurrence of mesoscopic disorder results in the appearance of first-order phase transitions between the states with different levels of atomic imbalance. The existence of a nonuniform external potential, such as trapping potential, essentially changes the lattice properties, suppressing the disorder fraction and rising the transition temperature.

1 Introduction

Optical lattices provide a convenient tool for modelling various many-body periodic structures [1-4]. The attractiveness of optical lattices is caused by the possibility of changing their properties in a required way. Thus, the lattice period, the depth of potential wells at lattice sites, and the lattice geometry, all these characteristics can be rather easily varied in experiment by applying the necessary laser beams. Also, the strength of atomic interactions can be regulated in a wide range by the Feshbach resonance techniques [5,6]. Respectively, it is feasible to create many artificial periodic structures with the properties necessary for different applications.

A special class of optical lattices is represented by the double-well lattices, where each lattice site is formed by a double-well potential [7-16]. Such lattices, similarly to single-well lattices, can be in superfluid or insulating state. In addition, they can exhibit other states that cannot arise in the single-well counterparts. For example, they can exhibit the ordered states with nonzero mean atomic imbalance and with phase transitions between the ordered state and a disordered state with zero average atomic imbalance [7-16]. Another unusual property of the double-well lattices is the possibility of forming mixed states, where mesoscopic regions of the ordered phase are intermixed with mesoscopic regions of the disordered phase [17]. In a bulk system, or in a sufficiently large trap, these regions are randomly distributed in space. While, for atoms in a tight trap, the region distribution is governed by the trap geometry. The latter would be similar to the radial distribution of superfluid fraction in a trap with a periodic crystalline-type atomic configuration [18].

The mixed state of a double-well optical lattice, with mesoscopic regions of different phases, exhibits a variety of interesting properties, distinguishing such a state from the purely ordered or completely disordered states. In our previous publication [17], we considered a rigid lattice with no external fields acting on the system. The aim of the present paper is twofold: to generalize the consideration by including external fields, and also to analyze the role of atomic vibrations in a double-well optical lattice. In Sec. 2, we derive a model of an insulating optical lattice in order to explain the physical meaning of all its terms and for explicitly demonstrating the origin of the term representing the influence of external potentials. In Sec. 3, atomic vibrations are introduced and their role in the renormalization of atomic interactions is analyzed. In Sec. 4, we study a double-well optical lattice with mesoscopic disorder in the presence of an external field. Section 5 contains conclusions and discussion.

Throughout the paper, we use the system of units with $\hbar = 1$ and $k_B = 1$.

2 Insulating Double-Well Optical Lattice

Deriving the model of a double-well optical lattice, we start with the standard Hamiltonian

$$\hat{H} = \int \psi^\dagger(\mathbf{r}) H_1(\mathbf{r}) \psi(\mathbf{r}) d\mathbf{r} + \frac{1}{2} \int \psi^\dagger(\mathbf{r}) \psi^\dagger(\mathbf{r}') \Phi(\mathbf{r} - \mathbf{r}') \psi(\mathbf{r}') \psi(\mathbf{r}) d\mathbf{r} d\mathbf{r}', \quad (1)$$

where $\psi(\mathbf{r})$ is a field operator of atoms, $\Phi(\mathbf{r})$ is a pair interaction potential, and in the single-atom Hamiltonian

$$H_1(\mathbf{r}) = -\frac{\nabla^2}{2m} + U(\mathbf{r}), \quad (2)$$

the external potential is a sum

$$U(\mathbf{r}) = V_L(\mathbf{r}) + U_{ext}(\mathbf{r}) ,$$

where the first term is the lattice potential, periodic with the lattice spacing \mathbf{a} , while the second term is not periodic, representing an additional external field, e.g., corresponding to a trapping potential. Atoms can be either bosons or fermions.

Keeping in mind an insulating lattice, the field operator can be expanded over an orthonormal basis of localized orbitals,

$$\psi(\mathbf{r}) = \sum_{nj} c_{nj} \psi_n(\mathbf{r} - \mathbf{r}_j) , \quad (3)$$

where n is a quantum multi-index and \mathbf{r}_j is a vector of atomic location. With this expansion, Hamiltonian (1) transforms to the expression

$$\hat{H} = \sum_{ij} \sum_{mn} E_{ij}^{mn} c_{mi}^\dagger c_{nj} + \frac{1}{2} \sum_{\{j\}} \sum_{\{n\}} \Phi_{j_1 j_2 j_3 j_4}^{n_1 n_2 n_3 n_4} c_{n_1 j_1}^\dagger c_{n_2 j_2}^\dagger c_{n_3 j_3} c_{n_4 j_4} , \quad (4)$$

in which

$$E_{ij}^{mn} \equiv \int \psi_m^*(\mathbf{r} - \mathbf{r}_i) H_1(\mathbf{r}) \psi_n(\mathbf{r} - \mathbf{r}_j) d\mathbf{r} \quad (5)$$

and $\Phi_{j_1 j_2 j_3 j_4}^{n_1 n_2 n_3 n_4}$ are the matrix elements of the interaction potential. As localized orbitals, one can take maximally localized Wannier functions designed for double-well lattices [19].

Considering the lattice with unity filling factor, it is necessary to impose the no-double-occupancy constraint

$$\sum_n c_{nj}^\dagger c_{nj} = 1 , \quad c_{mj} c_{nj} = 0 . \quad (6)$$

And in the case of an insulating lattice, the no-hopping condition

$$c_{mi}^\dagger c_{nj} = \delta_{ij} c_{mj}^\dagger c_{nj} \quad (7)$$

is valid. Then Hamiltonian (4) becomes

$$\hat{H} = \sum_j \sum_{mn} E_{jj}^{mn} c_{mj}^\dagger c_{nj} + \frac{1}{2} \sum_{i \neq j} \sum_{\{n\}} V_{ij}^{n_1 n_2 n_3 n_4} c_{n_1 i}^\dagger c_{n_2 j}^\dagger c_{n_3 j} c_{n_4 i} , \quad (8)$$

in which

$$V_{ij}^{n_1 n_2 n_3 n_4} \equiv \Phi_{ijji}^{n_1 n_2 n_3 n_4} \pm \Phi_{ijij}^{n_1 n_2 n_3 n_4} ,$$

the upper sign corresponding to Bose and the lower, to Fermi statistics. In the sums over atomic locations, one has $i \neq j$. To simplify the notation, we shall omit in what follows this inequality, setting instead the condition

$$V_{jj}^{n_1 n_2 n_3 n_4} \equiv 0 .$$

Each lattice site is formed by a double-well potential. The hopping between different lattice sites is absent in an insulating lattice. But the tunneling between the wells of a double-well potential in the same site is, generally, present. Therefore, to take into account

the tunneling, it is necessary to consider minimally two energy levels. In what follows, we take two such lowest levels with $n = 1, 2$. The necessity of taking at least two quantum states distinguishes the case of the double-well lattice from that of a lattice with single-well sites. The usual situation is when the ground-state function is symmetric with respect to spatial inversion, while the next-level state is antisymmetric, so that

$$\psi_1(-\mathbf{r}) = \psi_1(\mathbf{r}) , \quad \psi_2(-\mathbf{r}) = -\psi_2(\mathbf{r}) .$$

Because of this property, the off-diagonal matrix elements, such as V_{ij}^{1112} or V_{ij}^{2221} , are exactly zero. Even if the above symmetry property does not hold, such off-diagonal matrix elements are usually much smaller than the diagonal ones of the type V_{ij}^{1111} , V_{ij}^{2222} , V_{ij}^{1221} , and V_{ij}^{1122} . The nonzero matrix elements enter the following formulas through the combinations

$$\begin{aligned} A_{ij} &\equiv \frac{1}{4} (V_{ij}^{1111} + V_{ij}^{2222} + 2V_{ij}^{1221}) , & B_{ij} &\equiv \frac{1}{2} (V_{ij}^{1111} + V_{ij}^{2222} - 2V_{ij}^{1221}) , \\ C_{ij} &\equiv \frac{1}{2} (V_{ij}^{2222} - V_{ij}^{1111}) , & I_{ij} &= -2V_{ij}^{1122} . \end{aligned} \quad (9)$$

The latter are symmetric with respect to the change of the indices:

$$A_{ij} = A_{ji} , \quad B_{ij} = B_{ji} , \quad C_{ij} = C_{ji} , \quad I_{ij} = I_{ji} .$$

Introducing the notations

$$\begin{aligned} K_{ij}^{mn} &\equiv \int \psi_m^*(\mathbf{r} - \mathbf{r}_i) \left(-\frac{\nabla^2}{2m} \right) \psi_n(\mathbf{r} - \mathbf{r}_j) d\mathbf{r} , \\ U_{ij}^{mn} &\equiv \int \psi_m^*(\mathbf{r} - \mathbf{r}_i) U(\mathbf{r}) \psi_n(\mathbf{r} - \mathbf{r}_j) d\mathbf{r} , \end{aligned} \quad (10)$$

and invoking the symmetry properties, we have

$$K_{jj}^{mn} = \delta_{mn} K_{jj}^{nn} , \quad (11)$$

which gives

$$E_{jj}^{mn} = \delta_{mn} K_{jj}^{nn} + U_{jj}^{mn} . \quad (12)$$

The matrix elements of the kinetic energy can be represented as

$$\frac{\mathbf{p}_j^2}{2m} \equiv \frac{1}{2} (K_{jj}^{11} + K_{jj}^{22}) . \quad (13)$$

Also, we define

$$E_0 \equiv \frac{1}{2} \sum_j (E_{jj}^{11} + E_{jj}^{22}) = \sum_j \frac{\mathbf{p}_j^2}{2m} + U_0 N , \quad (14)$$

where

$$U_0 \equiv \frac{1}{2N} \sum_j (U_{jj}^{11} + U_{jj}^{22}) . \quad (15)$$

The quantity

$$H_j \equiv -E_{jj}^{12} - E_{jj}^{21} = -U_{jj}^{12} - U_{jj}^{21} \quad (16)$$

plays the role of an external field acting on the atom in a j -th lattice site. And

$$\Omega_j \equiv E_{jj}^{22} - E_{jj}^{11} + \sum_i C_{ij} \quad (17)$$

has the meaning of the tunneling frequency characterizing atomic tunneling between the wells of a double well. Depending on the shape of the double-well potential, this frequency can be varied in a wide range [20].

Then we use the operator transformation

$$\begin{aligned} c_{1j}^\dagger c_{1j} &= \frac{1}{2} + S_j^x, & c_{2j}^\dagger c_{2j} &= \frac{1}{2} - S_j^x, \\ c_{1j}^\dagger c_{2j} &= S_j^z - iS_j^y, & c_{2j}^\dagger c_{1j} &= S_j^z + iS_j^y. \end{aligned} \quad (18)$$

The operators

$$\begin{aligned} S_j^x &= \frac{1}{2} (c_{1j}^\dagger c_{1j} - c_{2j}^\dagger c_{2j}), & S_j^y &= \frac{i}{2} (c_{1j}^\dagger c_{2j} - c_{2j}^\dagger c_{1j}), \\ S_j^z &= \frac{1}{2} (c_{1j}^\dagger c_{2j} + c_{2j}^\dagger c_{1j}) \end{aligned} \quad (19)$$

satisfy spin algebra, independently from the statistics of atoms, whether Bose or Fermi. Because of their spin algebra, these operators are called pseudospin operators. With these notations, Hamiltonian (8) reduces to the form

$$\hat{H} = E_0 - \sum_j (\Omega_j S_j^x + H_j S_j^z) + \sum_{ij} \left(\frac{1}{2} A_{ij} + B_{ij} S_i^x S_j^x - I_{ij} S_i^z S_j^z \right). \quad (20)$$

According to their properties, the operator S_j^x describes atomic tunneling between the wells of a double-well potential in a j -th lattice site. The operator S_j^y corresponds to the Josephson current between the wells. And the operator S_j^z characterizes atomic imbalance of these wells [14-17].

3 Vibrating Double-Well Optical Lattice

Atoms, forming the lattice, are, of course, not immovable, but can vibrate around their lattice sites. In this section, we study the role of such vibrations.

Each atomic vector \mathbf{r}_j can be represented as the sum

$$\mathbf{r}_j = \mathbf{a}_j + \mathbf{u}_j \quad (21)$$

of the mean atomic location

$$\mathbf{a}_j \equiv \langle \mathbf{r}_j \rangle \quad (22)$$

and an atomic deviation from the mean location, such that

$$\langle \mathbf{u}_j \rangle = 0. \quad (23)$$

The latter condition follows directly from definitions (21) and (22).

The interaction matrix elements (9) are functions of the atomic vectors, so that, for instance,

$$A_{ij} \equiv A(\mathbf{r}_{ij}) \quad (\mathbf{r}_{ij} \equiv \mathbf{r}_i - \mathbf{r}_j) , \quad (24)$$

and, similarly, all other matrix elements (9). Since we are considering an insulating lattice, the atomic deviations are supposed to be small, because of which the interaction matrix elements can be expanded in powers of these deviations, limiting the expansions by the second-order terms, e.g., as

$$A_{ij} \cong A(\mathbf{a}_{ij}) + \sum_{\alpha} A_{ij}^{\alpha} u_{ij}^{\alpha} - \frac{1}{2} \sum_{\alpha\beta} A_{ij}^{\alpha\beta} u_{ij}^{\alpha} u_{ij}^{\beta} , \quad (25)$$

where the relative deviation is

$$\mathbf{u}_{ij} \equiv \mathbf{u}_i - \mathbf{u}_j \quad (26)$$

and the notations are used:

$$A_{ij}^{\alpha} \equiv \frac{\partial A(\mathbf{a}_{ij})}{\partial a_i^{\alpha}} \quad (\mathbf{a}_{ij} \equiv \mathbf{a}_i - \mathbf{a}_j) ,$$

$$A_{ij}^{\alpha\beta} \equiv \frac{\partial^2 A(\mathbf{a}_{ij})}{\partial a_i^{\alpha} \partial a_j^{\beta}} = - \frac{\partial^2 A(\mathbf{a}_{ij})}{\partial a_i^{\alpha} \partial a_i^{\beta}} .$$

In order to guarantee the validity of condition (23), one has to introduce the grand Hamiltonian

$$H = \hat{H} - \sum_j \Lambda_j \cdot \mathbf{u}_j , \quad (27)$$

with the Lagrange multipliers Λ_j cancelling in the Hamiltonian the terms linear in u_j^{α} . Then, expanding the matrix elements in powers of the relative deviations (26), we come to the grand Hamiltonian

$$H = U_0 N + \sum_j \left(\frac{\mathbf{p}_j^2}{2m} - \Omega_j S_j^x - H_j S_j^z \right) + \sum_{ij} \left\{ \frac{1}{2} A(\mathbf{a}_{ij}) - \frac{1}{4} \sum_{\alpha\beta} A_{ij}^{\alpha\beta} u_{ij}^{\alpha} u_{ij}^{\beta} + \right. \\ \left. + \left[B(\mathbf{a}_{ij}) - \frac{1}{2} \sum_{\alpha\beta} B_{ij}^{\alpha\beta} u_{ij}^{\alpha} u_{ij}^{\beta} \right] S_i^x S_j^x - \left[I(\mathbf{a}_{ij}) - \frac{1}{2} \sum_{\alpha\beta} I_{ij}^{\alpha\beta} u_{ij}^{\alpha} u_{ij}^{\beta} \right] S_i^z S_j^z \right\} . \quad (28)$$

To make the problem treatable, one needs to decouple the vibrational and atomic degrees of freedom. We use the following decoupling:

$$u_{ij}^{\alpha} u_{ij}^{\beta} S_i^{\gamma} S_j^{\gamma} = \langle u_{ij}^{\alpha} u_{ij}^{\beta} \rangle S_i^{\gamma} S_j^{\gamma} + u_{ij}^{\alpha} u_{ij}^{\beta} \langle S_i^{\gamma} S_j^{\gamma} \rangle - \langle u_{ij}^{\alpha} u_{ij}^{\beta} \rangle \langle S_i^{\gamma} S_j^{\gamma} \rangle . \quad (29)$$

The existence of atomic vibrations leads to the renormalization of atomic interactions. In turn, atomic interactions renormalize the phonon matrix

$$\Phi_{ij}^{\alpha\beta} \equiv A_{ij}^{\alpha\beta} + 2B_{ij}^{\alpha\beta} \langle S_i^x S_j^x \rangle - 2I_{ij}^{\alpha\beta} \langle S_i^z S_j^z \rangle . \quad (30)$$

The renormalized atomic interactions are

$$\tilde{B}_{ij} \equiv B(\mathbf{a}_{ij}) + \sum_{\alpha\beta} B_{ij}^{\alpha\beta} \langle u_i^{\alpha} u_j^{\beta} - u_j^{\alpha} u_j^{\beta} \rangle ,$$

$$\tilde{I}_{ij} \equiv I(\mathbf{a}_{ij}) + \sum_{\alpha\beta} I_{ij}^{\alpha\beta} \langle u_i^\alpha u_j^\beta - u_j^\alpha u_i^\beta \rangle . \quad (31)$$

Also, we introduce the notation

$$\tilde{E}_0 \equiv \left(\frac{A}{2} + U_0 \right) N + \sum_{ij} \sum_{\alpha\beta} \left(I_{ij}^{\alpha\beta} \langle S_i^z S_j^z \rangle - B_{ij}^{\alpha\beta} \langle S_i^x S_j^x \rangle \right) \langle u_i^\alpha u_j^\beta - u_j^\alpha u_i^\beta \rangle , \quad (32)$$

in which

$$A \equiv \frac{1}{N} \sum_{ij} A(\mathbf{a}_{ij}) . \quad (33)$$

As far as A is a constant, we have

$$\sum_i A_{ij}^{\alpha\beta} = - \frac{\partial^2 A}{\partial a_j^\alpha \partial a_j^\beta} = 0 , \quad \sum_{ij} A_{ij}^{\alpha\beta} u_j^\alpha u_j^\beta = \sum_i A_{ij}^{\alpha\beta} \sum_j u_j^\alpha u_j^\beta = 0 . \quad (34)$$

In the phonon matrix (30), the main term is $A_{ij}^{\alpha\beta}$. Therefore one has

$$\left| \sum_{ij} \Phi_{ij}^{\alpha\beta} u_j^\alpha u_j^\beta \right| \ll \left| \sum_{ij} \Phi_{ij}^{\alpha\beta} u_i^\alpha u_j^\beta \right| . \quad (35)$$

Thus, Hamiltonian (28) can be represented as the sum

$$H = \tilde{E}_0 + H_{ph} + H_{at} , \quad (36)$$

in which the first term is given by Eq. (32), the second term is the phonon Hamiltonian

$$H_{ph} = \sum_j \frac{\mathbf{p}_j^2}{2m} + \frac{1}{2} \sum_{ij} \sum_{\alpha\beta} \Phi_{ij}^{\alpha\beta} u_i^\alpha u_j^\beta , \quad (37)$$

and the third term is the atomic Hamiltonian

$$H_{at} = - \sum_j \left(\Omega_j S_j^x + H_j S_j^z \right) + \sum_{ij} \left(\tilde{B}_{ij} S_i^x S_j^x - \tilde{I}_{ij} S_i^z S_j^z \right) . \quad (38)$$

The phonon spectrum ω_{ks} is defined by the eigenvalue problem

$$\frac{1}{m} \sum_{j\beta} \Phi_{ij}^{\alpha\beta} e^{i\mathbf{k} \cdot \mathbf{a}_{ij}} e_{ks}^\beta = \omega_{ks}^2 e_{ks}^\alpha , \quad (39)$$

where \mathbf{e}_{ks} is a polarization vector, k is quasi-momentum, and s , polarization index. The phonon operators b_{ks} are introduced through the transformation

$$\begin{aligned} \mathbf{p}_j &= - \frac{i}{\sqrt{2N}} \sum_{ks} \sqrt{m\omega_{ks}} \mathbf{e}_{ks} \left(b_{ks} - b_{-ks}^\dagger \right) e^{i\mathbf{k} \cdot \mathbf{a}_j} , \\ \mathbf{u}_j &= \frac{1}{\sqrt{2N}} \sum_{ks} \frac{\mathbf{e}_{ks}}{\sqrt{m\omega_{ks}}} \left(b_{ks} + b_{-ks}^\dagger \right) e^{i\mathbf{k} \cdot \mathbf{a}_j} . \end{aligned} \quad (40)$$

Using this, the phonon Hamiltonian (37) becomes diagonal,

$$H_{ph} = \sum_{ks} \omega_{ks} \left(b_{ks}^\dagger b_{ks} + \frac{1}{2} \right) . \quad (41)$$

This allows us to find the deviation correlation function

$$\langle u_i^\alpha u_j^\beta \rangle = \frac{\delta_{ij}}{2N} \sum_{ks} \frac{e_{ks}^\alpha e_{ks}^\beta}{m\omega_{ks}} \coth \left(\frac{\omega_{ks}}{2T} \right) . \quad (42)$$

Since in the effective atomic interactions (31), we have $i \neq j$, they can be written as

$$\tilde{B}_{ij} = B(\mathbf{a}_{ij}) - \sum_{\alpha\beta} B_{ij}^{\alpha\beta} \langle u_j^\alpha u_j^\beta \rangle , \quad \tilde{I}_{ij} = I(\mathbf{a}_{ij}) - \sum_{\alpha\beta} I_{ij}^{\alpha\beta} \langle u_j^\alpha u_j^\beta \rangle . \quad (43)$$

And the nonoperator term (32) becomes

$$\tilde{E}_0 = \left(\frac{A}{2} + U_0 \right) N + \sum_{ij} \sum_{\alpha\beta} \left(B_{ij}^{\alpha\beta} \langle S_i^x S_j^x \rangle - I_{ij}^{\alpha\beta} \langle S_i^z S_j^z \rangle \right) \langle u_j^\alpha u_j^\beta \rangle . \quad (44)$$

The equation for the phonon spectrum (39) can be rewritten as

$$\omega_{ks}^2 = \frac{1}{m} \sum_j \sum_{\alpha\beta} \Phi_{ij}^{\alpha\beta} e_{ks}^\alpha e_{ks}^\beta e^{i\mathbf{k} \cdot \mathbf{a}_{ij}} . \quad (45)$$

For illustration, let us consider a lattice with cubic symmetry. Then we can define the effective spectrum ω_k through the average

$$\omega_k^2 \equiv \frac{1}{d} \sum_{s=1}^d \omega_{ks}^2 , \quad (46)$$

where d is space dimensionality. This yields

$$\omega_k^2 = - \frac{1}{m} \sum_j D_{ij} e^{i\mathbf{k} \cdot \mathbf{a}_{ij}} , \quad (47)$$

with the dynamical matrix

$$D_{ij} \equiv - \frac{1}{d} \sum_{\alpha=1}^d \Phi_{ij}^{\alpha\alpha} . \quad (48)$$

In the long-wave limit, using the property

$$\sum_j D_{ij} \cong 0 ,$$

we have

$$\omega_k^2 \simeq \frac{1}{2m} \sum_j D_{ij} (\mathbf{k} \cdot \mathbf{a}_{ij})^2 \quad (k \rightarrow 0) . \quad (49)$$

For a cubic lattice, the long-wave phonon spectrum reduces to

$$\omega_k \simeq ck \quad (k \rightarrow 0) , \quad (50)$$

with the sound velocity

$$c = \sqrt{\frac{Da^2}{2m}} , \quad (51)$$

and the isotropic dynamical matrix

$$D \equiv \frac{1}{a^2} \sum_j D_{ij} (a_{ij}^\alpha)^2 . \quad (52)$$

Here a is the lattice parameter of the cubic lattice.

It is important to emphasize that phonons can arise only in the presence of long-range atomic interactions. For example, in the case of local interactions [4], we have

$$\Phi_{ij} \approx U \exp(-q_0^2 a_{ij}^2) ,$$

where

$$a_{ij} \equiv |\mathbf{a}_{ij}| , \quad q_0 a \ll 1 ,$$

and U and q_0 are positive real parameters. This leads to

$$\Phi_{ij}^{\alpha\alpha} \approx 2q_0^2 \Phi_{ij} \left[1 - 2q_0^2 (a_{ij}^\alpha)^2 \right] .$$

Then the dynamical matrix (48) is negative:

$$D_{ij} \approx -2q_0^2 \Phi_{ij} \quad (\Phi_{ij} > 0) ,$$

which makes it impossible to define a real phonon frequency.

If Φ_{ij} is not Gaussian, but simply exponential, as

$$\Phi_{ij} \approx U \exp(-\mathbf{q}_0 \cdot \mathbf{a}_{ij}) \quad (U > 0) ,$$

then

$$\Phi_{ij}^{\alpha\alpha} \approx -(q_0^\alpha)^2 \Phi_{ij} ,$$

and the dynamical matrix is positive:

$$D_{ij} \approx \frac{1}{d} q_0^2 \Phi_{ij} \quad (\Phi_{ij} > 0) ,$$

making well defined a real phonon frequency.

When the interactions are of power law, as

$$\Phi_{ij} \approx \frac{U}{a_{ij}^n} \quad (n > 0) ,$$

then

$$\Phi_{ij}^{\alpha\alpha} \approx \frac{n\Phi_{ij}}{a_{ij}^2} \left[1 - \frac{(n+2)(a_{ij}^\alpha)^2}{a_{ij}^2} \right] .$$

The latter, for nearest neighbors, gives

$$D_{ij} \approx \frac{n\Phi_{ij}}{a^2} \left(\frac{n+2}{d} - 1 \right) .$$

Real phonon spectrum exists for a positive dynamical matrix D_{ij} . This means that the power law requires the condition

$$n > d - 2 .$$

If the lattice is sufficiently large, one can resort to the replacement of the summation over momenta by the integration over the Brillouin zone \mathcal{B} , so that

$$\frac{1}{V} \sum_k \longrightarrow \int_{\mathcal{B}} \frac{d\mathbf{k}}{(2\pi)^d} .$$

Then, from Eq. (43), we have

$$\langle u_j^\alpha u_j^\beta \rangle = \frac{\delta_{\alpha\beta}}{2m\rho} \int_{\mathcal{B}} \frac{1}{\omega_k} \coth\left(\frac{\omega_k}{2T}\right) \frac{d\mathbf{k}}{(2\pi)^d} . \quad (53)$$

This defines the mean square deviation

$$r_0^2 \equiv \sum_{\alpha=1}^d \langle u_j^\alpha u_j^\alpha \rangle = \langle u_j^\alpha u_j^\alpha \rangle d . \quad (54)$$

In this way, the effective atomic interactions (43), for a cubic lattice, become

$$\tilde{B}_{ij} = B(\mathbf{a}_{ij}) - \frac{r_0^2}{d} \sum_{\alpha} B_{ij}^{\alpha\alpha} , \quad \tilde{I}_{ij} = I(\mathbf{a}_{ij}) - \frac{r_0^2}{d} \sum_{\alpha} I_{ij}^{\alpha\alpha} , \quad (55)$$

which shows how atomic vibrations change the interaction of atoms.

4 Double-Well Lattice with Mesoscopic Disorder

Atomic vibrations can be called *microscopic* fluctuations, since they are related to the fluctuations of separate atoms around their lattice sites. As is shown in the previous section, such fluctuations renormalize the strength of atomic interactions.

There exists another type of fluctuations, whose occurrence can lead to a much more noticeable change of system properties. These fluctuations are termed *mesoscopic*, because each fluctuation involves many atoms that move coherently. The fluctuations are called mesoscopic, since their typical linear size is much larger than the mean interatomic distance, but smaller than the system size. These fluctuations represent strong fluctuations of order parameters, as a result of which the system can be treated as a fluctuating mixture of different thermodynamic phases, say, an ordered and a disordered phase. Then the appearance of such mesoscopic fluctuations of competing phases can be understood as the occurrence of mesoscopic disorder. This type of fluctuations can lead to an essential change of system properties, as has been demonstrated for several kinds of matter of different physical nature, e.g., for ferromagnets [21,22], antiferromagnets [23,24], ferroelectrics [25], crystals [26], and

other materials reviewed in Ref. [27]. A somewhat close behavior happens for the clustering nuclear matter [28,29].

In our previous paper [17], we have considered the influence of such mesoscopic disorder on double-well optical lattices, when there are no external fields. In the present section, we generalize the consideration to the case of a nonzero external field. The latter can be caused, e.g., by the presence of a trapping potential. We study a fluctuating mixture of two phases, an ordered phase, where there exists an average large atomic imbalance between the wells of double-well potentials, and a disordered phase, where such an imbalance is small. In the absence of external fields, the atomic imbalance of the disordered phase is exactly zero.

After averaging over various configurations, produced by mesoscopic fluctuations, as described in Refs. [17,27], we have, instead of Eq. (20), the effective Hamiltonian

$$\tilde{H} = \hat{H}_1 \oplus \hat{H}_2 , \quad (56)$$

in which each term

$$H_\nu = w_\nu E_0 - w_\nu \sum_j (\Omega_j S_j^x + H_j S_j^z) + w_\nu^2 \sum_{i \neq j} \left(\frac{1}{2} A_{ij} + B_{ij} S_i^x S_j^x - I_{ij} S_i^z S_j^z \right) \quad (57)$$

corresponds to the related phase labelled by the index $\nu = 1, 2$. Each Hamiltonian part (57) acts on a weighted Hilbert space \mathcal{H}_ν . And the total Hamiltonian (56) is defined on the fiber space

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 . \quad (58)$$

The geometric weights w_ν of the phases are defined as the minimizers of the thermodynamic potential

$$F = -T \ln \text{Tr} e^{-\beta \tilde{H}} , \quad (59)$$

under the normalization condition

$$w_1 + w_2 = 1 , \quad 0 \leq w_\nu \leq 1 .$$

The quantities of interest are the average values of the tunneling intensity

$$x_\nu \equiv \frac{2}{N} \sum_j \langle S_j^y \rangle_\nu , \quad (60)$$

Josephson current

$$y_\nu \equiv \frac{2}{N} \sum_j \langle S_j^y \rangle_\nu , \quad (61)$$

and the mean atomic imbalance

$$s_\nu \equiv \frac{2}{N} \sum_j \langle S_j^z \rangle_\nu . \quad (62)$$

Here the index ν in the statistical averages implies the averaging with respect to Hamiltonian (57). The atomic imbalance (62) plays the role of an order parameter distinguishing an ordered and a disordered phases. This definition implies the constraint

$$s_1 > s_2 . \quad (63)$$

When external fields are switched off, the order parameter of the disordered phase has to be zero, which assumes the limiting condition

$$\lim_{\{H_j \rightarrow 0\}} s_2 = 0 . \quad (64)$$

To calculate the above quantities (60), (61), and (62), we need to invoke some approximation for the Hamiltonian terms containing pairs of pseudospins. For this purpose, we resort to the Kirkwood approximation [30], according to which for a pair of operators, acting on the space \mathcal{H}_ν , one has the decoupling

$$S_i^\alpha S_j^\beta = g_{ij}^\nu \left(\langle S_i^\alpha \rangle_\nu S_j^\beta + S_i^\alpha \langle S_j^\beta \rangle_\nu - \langle S_i^\alpha \rangle_\nu \langle S_j^\beta \rangle_\nu \right) \quad (i \neq j) , \quad (65)$$

in which g_{ij}^ν is a pair correlation function and the index ν at the angle brackets means the statistical averaging with the related Hamiltonian (57). This decoupling differs from the mean-field approximation by the presence of the pair correlation function.

In the formulas below, we shall employ the notations for the average interaction intensities

$$B_\nu \equiv \frac{1}{N} \sum_{i \neq j} g_{ij}^\nu B_{ij} , \quad I_\nu \equiv \frac{1}{N} \sum_{i \neq j} g_{ij}^\nu I_{ij} . \quad (66)$$

We assume that the trap is sufficiently wide, so that the quantities

$$\Omega_j = \Omega \quad H_j = H_0 \quad (67)$$

can be treated as independent from the lattice indices. Also, we introduce the notations

$$\tilde{E}_\nu \equiv w_\nu E_0 + w_\nu^2 \frac{N}{2} \left(A - \frac{B_\nu}{2} x_\nu^2 + \frac{I_\nu}{2} s_\nu^2 \right) \quad (68)$$

and

$$\tilde{\Omega}_\nu \equiv w_\nu \Omega - w_\nu^2 B_\nu x_\nu , \quad \tilde{I}_\nu \equiv w_\nu H_0 + w_\nu^2 I_\nu s_\nu . \quad (69)$$

Then Hamiltonian (57) reduces to the form

$$\hat{H}_\nu = \tilde{E}_\nu - \sum_j \left(\tilde{\Omega}_\nu S_j^x + \tilde{I}_\nu S_j^z \right) . \quad (70)$$

For the thermodynamic potential (59), we find

$$F = F_1 + F_2 , \quad F_\nu = \tilde{E}_\nu - NT \ln \left(2 \cosh \frac{J_\nu}{2T} \right) , \quad (71)$$

where

$$J_\nu \equiv \sqrt{\tilde{\Omega}_\nu^2 + \tilde{I}_\nu^2} . \quad (72)$$

The tunneling intensity (60) becomes

$$x_\nu = \frac{\tilde{\Omega}_\nu}{J_\nu} \tanh \left(\frac{J_\nu}{2T} \right) . \quad (73)$$

The Josephson current (61) in an equilibrium system is zero,

$$y_\nu = 0 . \quad (74)$$

And the atomic imbalance (62) reads as

$$s_\nu = \frac{\tilde{I}_\nu}{J_\nu} \tanh \left(\frac{J_\nu}{2T} \right) . \quad (75)$$

In order to estimate the relation between the different interaction terms (9), we can take into account that the values V_{ij}^{1111} , V_{ij}^{2222} and V_{ij}^{1221} are close to each other, so that we can set

$$V_{ij}^{1111} = V_{ij}^{2222} = V_{ij}^{1221} \equiv V_{ij} .$$

As a result,

$$A_{ij} = V_{ij} , \quad B_{ij} = 0 , \quad C_{ij} = 0 .$$

We shall use this simplification in what follows.

To accomplish numerical calculations, we need to define the pair correlation function. Here, for simplicity, we set

$$g_{ij}^\nu = 1 , \quad (76)$$

which reduces the Kirkwood approximation to the mean-field form. For the convenience of numerical calculations, we define the dimensionless thermodynamic potentials

$$G \equiv \frac{F}{NI} , \quad G_\nu \equiv \frac{F_\nu}{NI} , \quad (77)$$

in which

$$I \equiv \frac{1}{N} \sum_{i \neq j} I_{ij} = I_\nu . \quad (78)$$

It is also convenient to introduce the dimensionless parameters

$$u \equiv \frac{A}{I} , \quad \omega \equiv \frac{\Omega}{I} , \quad h \equiv \frac{H_0}{I} . \quad (79)$$

Then for quantities (69) and (72), we have

$$\frac{\tilde{\Omega}_\nu}{I} = w_\nu \omega , \quad \frac{J_\nu}{I} = w_\nu f_\nu , \quad \frac{\tilde{I}_\nu}{I} = w_\nu h + w_\nu^2 s_\nu , \quad (80)$$

where

$$f_\nu \equiv \sqrt{(h + w_\nu s_\nu)^2 + \omega^2} . \quad (81)$$

Measuring temperature in units of I , for the tunneling intensity (73), we get

$$x_\nu = \frac{\omega}{f_\nu} \tanh \left(\frac{w_\nu f_\nu}{2T} \right) , \quad (82)$$

while the atomic imbalance (75) becomes

$$s_\nu = \frac{h + w_\nu s_\nu}{f_\nu} \tanh \left(\frac{w_\nu f_\nu}{2T} \right) . \quad (83)$$

In the dimensionless notation, the thermodynamic potential (77) reads as

$$G = G_1 + G_2, \quad G_\nu = e_\nu - T \ln \left[2 \cosh \left(\frac{w_\nu f_\nu}{2T} \right) \right], \quad (84)$$

with

$$e_\nu = w_\nu \frac{E_0}{NI} + \frac{w_\nu^2}{4} (2u + s_\nu^2). \quad (85)$$

Recall that, in addition to the above equations, we have to define the geometric weights of the ordered and disordered phases as the minimizers of the thermodynamic potential G . To take explicitly into account the normalization condition, we introduce the notation

$$w \equiv w_1, \quad w_2 = 1 - w. \quad (86)$$

Minimizing the thermodynamic potential (84) with respect to w , we find the equation

$$w = \frac{2u + \omega(x_1 - x_2) + h(s_1 - s_2) - s_2^2}{4u - s_1^2 - s_2^2}, \quad (87)$$

defining the weight of the ordered phase. The weight of the disordered phase, according to relation (86), is $1 - w$.

When the gap between the energy levels E_{jj}^{11} and E_{jj}^{22} , defined in Eq. (5), is small, as compared to the interaction intensity (78), then, in view of definition (17), one has $\omega \ll 1$. In that case, we have

$$f_\nu = h + w_\nu s_\nu, \quad x_\nu = 0 \quad (\omega \rightarrow 0),$$

$$s_\nu = \tanh \left[\frac{w_\nu (h + w_\nu s_\nu)}{2T} \right].$$

Therefore, the atomic imbalance for the ordered phase becomes

$$s_1 = \tanh \left(\frac{wh + w^2 s_1}{2T} \right). \quad (88)$$

The atomic imbalance for the disordered phase is

$$s_2 = \tanh \left(\frac{(1-w)h + (1-w)^2 s_2}{2T} \right). \quad (89)$$

And the equation (87) for the geometric weight of the ordered phase takes the form

$$w = \frac{2u + h(s_1 - s_2) - s_2^2}{4u - s_1^2 - s_2^2}. \quad (90)$$

These are the main equations we need to solve, keeping in mind constraints (63) and (64). In addition, we have to compare the thermodynamic potential of the mixed system, (84), with that of a pure ordered system, when $w = 1$ and there exists just one order parameter s_1 given by the equation

$$s_1 = \tanh \left(\frac{s_1 + h}{2T} \right).$$

Note that there always exists a solution with $w = 0.5$ representing a degenerate case, when the competing phases are asymptotically equivalent. Among all possible solutions, we have to select the most stable one, which minimizes the system thermodynamic potential and satisfies all imposed constraints, such as Eqs. (63) and (64) and the condition $0 \leq w \leq 1$. The solution $w = 0$ makes the value s_1 undefined, hence constraint (63) inapplicable. Therefore this case is unphysical and has to be excluded.

The results of numerical calculations are presented in Figs. 1 and 2. The parameters u and h have been varied in a wide range. When $u \leq 0$, the most stable solution corresponds to the pure system, with no mesoscopic disorder and $w = 1$ for all temperatures. Positive values of u allow for the appearance of mesoscopic disorder. According to definition (79), the positive parameter u can be interpreted as the ratio of the disordering interaction strength A to the ordering interaction strength I . Thence this ratio u can be called the disordering parameter. It turns out that for $u > 0.5$ the solutions are not continuous. This could mean that such a strong disorder parameter prohibits the states with mesoscopic fluctuations, at least in the frame of the present model. To consider the higher values of u requires to invoke a more sophisticated approximation than the mean-field one. Varying u in the interval $0 < u < 0.5$ shows that at $T = 0$, we have $s_1 = 1$ and the most stable is the state with $w = 1$. With rising temperature, the state with $w = 1$ and $s_2 = 0$ persists till the transition temperature T_0 , where there occurs a first-order phase transition to the state with $w = 0.5$. The transition temperatures, as functions of u and h , are depicted in Fig 1. The behavior of the order parameter s_1 is presented in Fig 2 for different values of u and h .

5 Discussion

The influence of atomic vibrations and mesoscopic disorder on the properties of an insulating double-well optical lattice are studied. Atomic vibrations result in the appearance of well-defined phonon degrees of freedom, provided that the interactions between atoms are sufficiently long-ranged. For example, local interactions, described by a delta-function potential, typical of many rarified trapped gases, do not allow for the formation of well-defined phonons, since their spectrum turns out to be imaginary. But long-range interactions, such as existing between atoms with electric or magnetic dipoles, perfectly allow for the appearance of well-defined phonon degrees of freedom. At the present time, several atomic species are known, enjoying such long-range dipole interactions, for instance, ^{52}Cr possessing large magnetic moments [31,32], Rydberg atoms [33] and polar molecules [34].

So, the consideration of the present paper concerns this type of dipolar gases loaded into an optical lattice. We show that atomic vibrations in a double-well optical lattice renormalize the strength of atomic interactions.

Atomic vibrations can be called *microscopic* fluctuations, since they correspond to the oscillations of separate atoms, though interacting with each other, but the motion of atoms being not correlated. There exists another kind of fluctuations, when atoms move in a coherent manner, locally defining an order parameter that differs from that of the surrounding matter. The typical size of such a coherent atomic group is intermediate between the mean interatomic distance and the linear system size, because of which these coherent oscillations are termed *mesoscopic*. When the latter correspond to the order parameters of different thermodynamic phases, these oscillations can be called *heterophase*. Such mesoscopic fluc-

tuations can occur in various statistical systems of condensed-matter type [21-27] and in many macromolecular systems [35].

Mesoscopic fluctuations can also occur in double-well optical lattices [17]. Here, an ordered state corresponds to a nonzero atomic imbalance between the wells of the double wells. If there are no external fields, the disordered state is characterized by zero atomic imbalance [17]. But in the presence of external fields, disorder corresponds to an atomic imbalance that is not exactly zero, but smaller than the imbalance in the ordered state. We have generalized the previous analysis of mesoscopic disorder in a lattice without external fields to the case of nonzero external fields that can be related, e.g., to the presence of a trapping potential. The existence of external fields essentially changes the system properties, leading to the occurrence of first-order phase transitions between the states with different order parameters, that is, between the states with different atomic imbalance.

It is worth noting that term (16), corresponding to an external field, arises only when, in addition to the lattice potential, there is a nonuniform external potential, such as trapping potential. To show this, let us consider an ideal optical lattice with a periodic potential

$$U(\mathbf{r}) = U(\mathbf{r} + \mathbf{a}_j) .$$

In that case, the single-atom Hamiltonian (2) enjoys Bloch waves as its eigenstates, defined by the eigenproblem

$$H_1(\mathbf{r})\varphi_{nk}(\mathbf{r}) = E_{nk}\varphi_{nk}(\mathbf{r}) .$$

Taking for atomic orbitals the well-localized Wannier functions [19], we have the relation

$$\psi_n(\mathbf{r} - \mathbf{a}_j) = \frac{1}{\sqrt{N}} \sum_k \varphi_{nk}(\mathbf{r}) e^{-i\mathbf{k} \cdot \mathbf{a}_j} .$$

Then for the matrix elements (5), we obtain

$$E_{ij}^{mn} = \frac{\delta_{mn}}{N} \sum_k E_{nk} e^{i\mathbf{k} \cdot \mathbf{a}_j} .$$

Thus, these matrix elements are purely diagonal with respect to the band indices m, n . Therefore, the effective field (16), caused by nondiagonal elements, is strictly zero, hence $h = 0$.

The occurrence of mesoscopic fluctuations, causing the appearance of mesoscopic disorder in a double-well optical lattice, changes the system properties in a much more dramatic way than microscopic fluctuations, such as atomic vibrations.

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Figure Captions

Fig. 1. Transition temperature T_0 in units of I : (a) as a function of h for different values of u ; (b) as a function of u for different values of h .

Fig. 2. Order parameter s_1 as a function of dimensionless temperature for different values of the disorder parameter: (a) $u = 0.1$; (b) $u = 0.5$. The lines are marked by the numbers corresponding to different values of the external field: (1) $h = 0$; (2) $h = 0.2$; (3) $h = 0.4$; (4) $h = 0.6$; (5) $h = 0.8$; (6) $h = 1.0$.

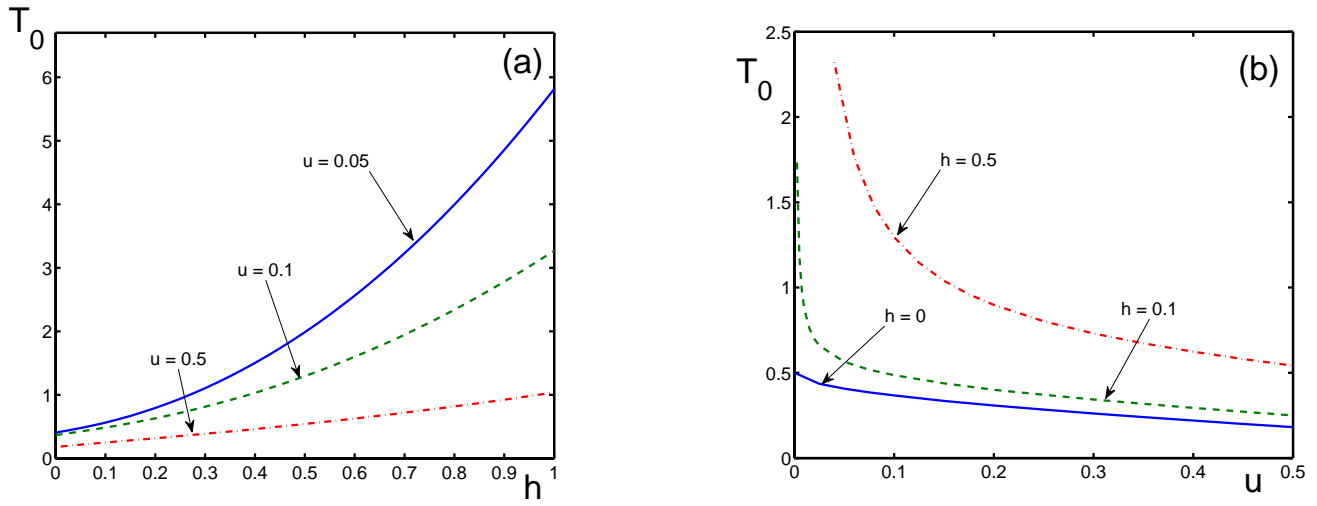


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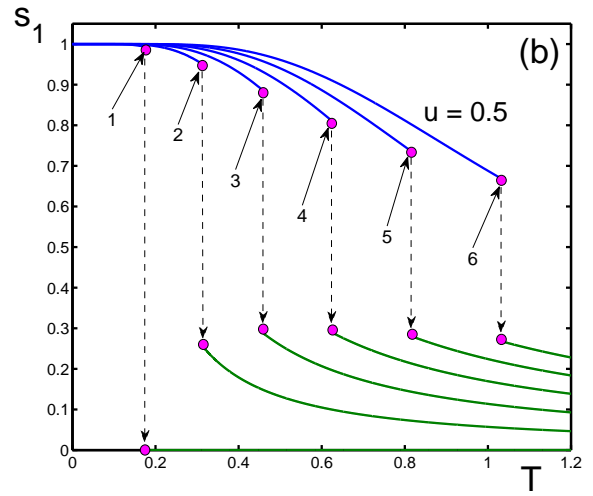
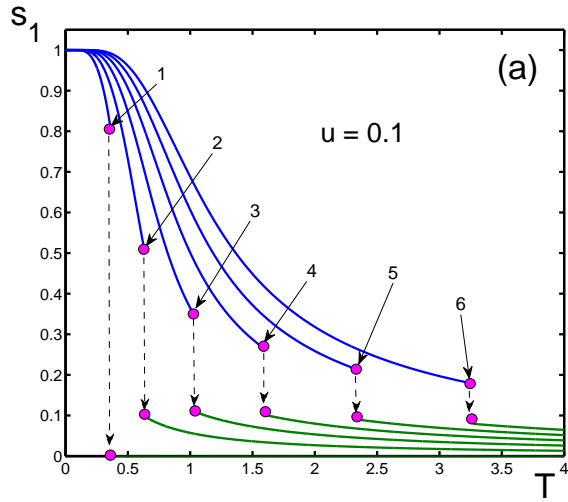


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